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EFFECT OF AN ELECTRIC FIELD ON A SPLIT BLOCH BAND

by

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The effect of a constant and uniform electric field on a split Bloch band is studied. We show how the Wannier-Stark ladders of the parent band is modified by a potential in addition to that of the crystal. We examine how the frequency spectrum behaves as the field strength varies from weak to strong. In the case that the parent band is split into a finite number of sub-bands, we show that there exists a set of subspaces to which the states return periodically in time, and that the constituent states of each subspace are localized around a given unit cell. We develop a theoretical framework which naturally exploits the symmetries of the system and which also allows for easy and clean numerical calculations.

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Effect of an electric field on a split Bloch band

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ABSTRACT: The effect of a constant and uniform electric field on a split Bloch band is studied through a tight binding model. We show how the Wannier-Stark ladders of the parent band is modified by a potential in addition to that of the crystal. We examine how the frequency spectrum behaves as the field strength varies from weak to strong. In the case that the parent band is split into a finite number of sub-bands, we show that there exists a set of subspaces to which the states return periodically in time, and that the constituent states of each subspace are localized around a given unit cell. We develop a theoretical framework which naturally exploits the symmetries of the system and which also allows for easy and clean numerical calculations.

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1. Introduction

Nearly three decades ago Wannier proposed that the electronic Bloch states of a crystalline solid become sets of new states, later called Wannier-Stark (WS) ladders, when a constant and uniform electric field is applied.[1] This has generated an intensive research field with lasting interest. There has been some controversy about the very existence of such states,[2] but it has been made clear that the notion of WS ladders is valid if a finite number of Bloch bands are considered, with their couplings with the rest of the states ignored.[3] The criterion for ignoring the coupling between two bands is that they are separated by a gap which is large, such that the process of Zener tunneling is sufficiently slow to be considered unimportant at least from a dynamical point of view.[4] Some of the basic properties of the WS ladders have been observed experimentally.[5]

In the simple case where a given Bloch band can be regarded as decoupled from the others, the nature of the associated WS ladders has been known quite well.[6] A number of discussions have been made regarding the choice of different gauge and boundary conditions, all revealing the basic structure of the frequency spectrum: uniformly spaced levels with spacing $Fa/\hbar$, where F is the electric force and a the lattice constant in the field direction. In a static representation of the field, the eigenenergies are found to be uniformly spaced with spacing Fa, and the eigenenergy states are found to be localized more than exponential functions. In a vector potential representation of the field, where the Hamiltonian is no longer time independent, a complete set of solutions, known as Houston functions, is found for the time dependent Schrodinger equation. The Houston functions are essentially the Bloch functions with the crystal momentum drifting with a constant speed, F, in the field direction. The Bloch oscillation, namely the periodic recurrence of the the Houston functions when the crystal momentum transverses the Brillouin zone, then gives rise to the uniformly spaced frequency levels. In fact, it has been shown that *any*

initial state in a given band will return itself in a period of Bloch oscillation (see Luban in ref.6).

In this paper we study the effect of an electric field on an isolated Bloch band which is split by a potential in addition to that of the crystal. By *isolated* we mean that the spectral range under consideration is bounded by large energy gaps, such that the splitting potential and the field do not mix it significantly with the rest of the spectrum. This is clearly a situation that can be realized in an experiment. In particular, we think of a superlattice which modulates the solid in one of the crystal directions, with the electric field applied in the same direction.[7] As far as the motion in the field direction is concerned, the system can be ideally modeled by an one dimensional tight binding chain. For simplicity, we will take the hopping amplitudes to be nonzero between nearest neighbors only and to be independent of positions. The splitting potential will be represented by a set of position dependent site energies.

We wish to investigate the following issues. First, we would like to show analytically how the WS ladders of the parent band be modified under a weak but otherwise arbitrary potential. From a point of view that the pieces of the split spectrum are going to be strongly coupled together by even a moderate field, the solution of this problem should shed some light on a strongly coupled multi-band system. Secondly, when the potential is periodic (weak or strong) but not constant, the parent band is split into a finite number of sub-bands. In this case it is known that there will be n sets of WS ladders under a field, where n is the number of sub-bands. We would like to examine how the energy (frequency) levels in different sets are placed relative to one another, and to show how their positions vary as functions of the field strength or other parameters. We would like to see the behavior of the ladders in the extremes of weak and strong fields, and to see how the behavior changes from one extreme to the other. Also, we are interested to know what can happen when a pair of sub-bands become degenerate. Thirdly, about the time

evolution of the system, we would like to show a generalized periodic recurrence of the states, which has been expected in a single band approximation. Finally, we would like to develop a theoretical framework, which exploits the symmetries of the system and which allows for clean and easy numerical calculations.

There has been some studies of multi-band systems in the literature, but many of them considered the case of weak coupling limit.[1,4,6,8,9] It is in this limit that the notion of metastability of the WS ladders has been extensively investigated.[9] The present work tries to go beyond the weak coupling limit, and to emphasize on the strong coupling regime. Fukuyama et al[10] have studied a tight binding model, in which arbitrary strength of couplings were taken into account, but only a pair of bands were included. There have also been a few numerical studies on finite size systems,[11] but a clear picture has not been obtained regarding the behavior of the WS ladders as functions of the field strength and etc. Finally we would like to mention a branch of research on the localization of the WS states,[12] where the regime of strong coupling has also been dealt with.

Having described the main scope of this work, we now proceed to outline our theoretical approach. When dealing with an electric field, one encounters the complication that it cannot be represented by gauge potentials which are uniform both in space and time, even if the field itself is uniform. Thus, one has to deal with a Hamiltonian which is either time dependent or lacks the symmetry of spatial translation that the Hamiltonian might have in the absence of the electric field. The difficulty has been reflected in the earlier work on WS ladders.[13] It is well known that the WS ladders have their origin in the spatial periodicity of the crystal potential, so it would be nice to utilize this symmetry explicitly in one's treatment. This can be achieved by using a vector potential to represent the field, but the Hamiltonian then becomes time dependent. The time dependence is not a problem if a single band approximation is used, but it can cause difficulty in a more accurate treatment of a multi-band system. Earlier utilization of the spatial symmetry has

been primarily limited to inferring some general structure of the WS ladders. Therefore, when calculating the spectrum or the states, one often took the static representation of the field and used fixed-end boundary conditions or alike. The boundary effect could then mix up the otherwise perfect structure of the WS ladders and make it difficult to determine how different sets of WS ladders place themselves.

This embarrassing situation can somehow be avoided, if it is realized that, when modified by appropriate gauge transformations, the space-time translations can still be symmetry operations of the Hamiltonian. In other words, one has to replace the space-time translations by their gauge covariant forms in order to reveal the physical symmetry associated with the uniformity of the electric field. These are the so called electric translations originally introduced by Ashby and Miller[14] in analogy with the symmetry of magnetic translations.[15] In this work, we will utilize the symmetry of electric translations to guide our general ideas. The actual formulation of our approach will, however, be made in an elementary fashion.

We will represent the electric field by a vector potential which is uniform in space and linear in time. We will take a periodic boundary condition in order to accommodate the symmetry of spatial translations that the system might have. The Hamiltonian is no longer time independent, so we will focus our attention on the evolution operator.[16] The symmetries of the electric translations will then give us valuable information about the frequency spectrum and the time evolution of the system.

With the above choice of gauge, the electric translations in space are the bare translations in space, and those in time are the combined time and momentum shifts (see (2.4) and (2.17)). As is true for the magnetic translations, the electric translations in space in general do not commute with those in time, unless the steps of spatial and time translations satisfy the following relation:

$$\delta_x \delta_t = \text{integer} \times h/F. \tag{1.1}$$

Due to this restriction, only subgroups of the electric translations can be diagonalized simultaneously with one another and with the evolution operator. The subsequent sections of this paper are basically organized according to three classifications of the symmetry subgroups, each emphasizing a different aspect of the system. The results obtained in different ways are related and complementary.

If we take the system size, Na, as the basic spatial step for a subgroup, then $h/(FaN)$ is the finest time step allowable. The consequence of the symmetries of this subgroup is the subject of study in section 2. When the site potential is periodic with period pa, it will be advantageous to consider a subgroup with pa as the basic spatial step. The finest time step allowable is then $h/(Fap)$. As will be shown in section 3, this subgroup of symmetry operations can yield a great deal of information about the time evolution of the system, such as the existence of a set of invariant subspaces in each of which the states are localized (more than exponential) around a given unit cell. The WS ladders will naturally manifest themselves through the periodic structure of the frequency spectrum. Section 4 can be regarded as an extension of section 3. A detailed investigation of the weak and strong field limits will be given there. The weak field limit is in fact an adiabatic limit, where one can see how the Berry phases[17] play their roles. Some numerical results for a discrete cosine potential will be given to illustrate ideas and to cover the intermediate field strengths. In section 5, we will consider yet another subgroup of electric translations. The basic time step will be taken as h/Fa, which is the period of Bloch oscillations of the parent band. The explicit time periodicity of the Schrodinger equation will be exploited by the application of the Floquet theorem. It is in this approach that weak perturbations of the WS ladders of the parent Bloch band can be conveniently studied. Examples will be given for a single impurity potential and for some periodic potentials.

In section 6, We will summarize our results, with some remarks regarding the generality of our approach.

2. Electric translation in time as a dynamical symmetry

In the simplest form, a Bloch band is described by the tight-binding Schrodinger equation

$$i\hbar\frac{\partial}{\partial t}\psi(n,t) = -R/2[\psi(n+1,t) + \psi(n-1,t)], \tag{2.1}$$

with a periodic boundary condition

$$\psi(n+N,t) = e^{i\alpha aN}\psi(n,t), \tag{2.2}$$

where R is the band width, and N the total number of sites. A constant phase factor has been inserted in the boundary condition for generality and for later reference. If the system is perturbed by a site potential V_n and an electric field, equation (2.1) is modified to the following form

$$i\hbar\frac{\partial}{\partial t}\psi(n,t) = -R/2[e^{iFat/\hbar}\psi(n+1,t) + e^{-iFat/\hbar}\psi(n-1,t)] + V_n\psi(n,t), \tag{2.3}$$

where F is the electrical force and a the lattice constant. The electric field has been represented by a time-dependent vector potential. This introduces a time dependence in the Hamiltonian, and therefore renders useless the convenient characterization of the system by energy eigenvalues and eigenstates. It is known that the time dependence can not be removed by any choice of gauge which conforms with the boundary condition (2.2). (Had we used a fixed-end boundary condition (see (2.22)), the time dependence can be removed by a gauge transformation $\psi'(n,t) = \exp(iFant/\hbar)\psi(n,t)$. In the new gauge, the field is represented by a static potential $-Fan$.) The motivation of insisting on a periodic boundary condition is, of course, to accommodate the symmetry of spatial translation that the system may have. It will be seen in the next section that the WS ladders can be presented most cleanly this way. Another advantage of using a periodic boundary condition is its convenience in dealing with transport problems. We would like to explore

what kind of dynamical symmetries still remain in the system, assuming at the moment a general static potential.

One obvious symmetry is the time periodicity in the Hamiltonian, which is associated with the Bloch oscillation of the parent band. A number of useful results can be obtained by utilizing the Floquet theorem applicable to linear differential equations with periodic coefficients. We will look into this in section 5.

What is not so obvious is the symmetry of the following type. Suppose $\psi(n,t;\alpha)$ is a solution of (2.3) and (2.2), then

$$g_l(n,t;\alpha) \equiv e^{i2\pi nl/N}\psi(n,t+l\tau;\alpha),\ l = \text{integers} \tag{2.4}$$

are also solutions, where $\tau \equiv h/(FaN)$. This is the symmetry of a subgroup of *electric translations* that we talked about in the introduction. Because of the boundary condition (2.2), the basic time step cannot be smaller than $h/(FaN)$. In other words, the boundary condition implies a largest possible spatial step Na, the system size, such that the sizes of the time steps have to be bounded from zero according to (1.1).

It is convenient to introduce the evolution operator $\hat{U}(t,t';\alpha)$ for equation (2.3) with the boundary condition (2.2). By definition, if $\psi(n,t)$ is an arbitrary solution of (2.3) and (2.2), then

$$\psi(n,t) = \sum_{n'} \hat{U}_{nn'}(t,t';\alpha)\psi(n',t'). \tag{2.5}$$

The symmetry (2.4) implies that,

$$\begin{aligned} g_{l+1}(n,t;\alpha) &= e^{i2\pi n/N} g_l(n,t+\tau;\alpha) \\ &= e^{i2\pi n/N} \sum_{n'} \hat{U}_{nn'}(t+\tau,t;\alpha) g_l(n,t;\alpha). \end{aligned} \tag{2.6}$$

It is then clear that a state $\psi(n,t;\alpha)$ in the first time interval, $0 \le t < \tau$, is carried over to the subsequent intervals by repeated application of the operator $\bar{U}(t;\alpha)$, where

$$\bar{U}_{n,n'}(t;\alpha) \equiv e^{i2\pi n/N}\hat{U}_{nn'}(t+\tau,t;\alpha). \tag{2.7}$$

As a result, the system is completely described by $\hat{U}(t,0;\alpha)$ and $\bar{U}(t;\alpha)$ for $0 \leq t < \tau$.

We now proceed with a general analysis of the operators $\hat{U}$ and $\bar{U}$. Being the evolution operator of a Schrodinger equation with a Hermitian Hamiltonian, $\hat{U}$ is unitary and satisfies the following relations:

$$\begin{aligned} \hat{U}(t,t';\alpha) &= \hat{U}(t,t'';\alpha)\hat{U}(t'',t';\alpha), \\ \hat{U}(t,t';\alpha) &= \hat{U}^{\dagger}(t',t;\alpha), \end{aligned} \tag{2.8}$$

where t, t' and t'' are arbitrary time instants. The α periodicity of the boundary condition (2.2) implies that

$$\hat{U}(t,t';\alpha + 2\pi/(Na)) = \hat{U}(t,t';\alpha). \tag{2.9}$$

Moreover, it can be shown that

$$\hat{U}(t,t';\alpha) = e^{i\alpha a\hat{n}}\hat{U}(t + \hbar\alpha/F, t' + \hbar\alpha/F; 0)e^{-i\alpha a\hat{n}}, \tag{2.10}$$

which is true for any Hamiltonian that is independent of time in the absence of the electric field, where $\hat{n}$ is the site position operator. Using these general relations and the definition in (2.7), we can now show that

$$\begin{aligned} & e^{-i\alpha a\hat{n}}\bar{U}(t;\alpha)e^{i\alpha a\hat{n}} \\ &= e^{i2\pi\hat{n}/N}\hat{U}(t + \tau + \hbar\alpha/F, t + \hbar\alpha/F; 0) \\ &= e^{i2\pi\hat{n}/N}\hat{U}(t + \tau + \hbar\alpha/F, \tau; 0)\hat{U}(\tau, 0; 0)\hat{U}(0, t + \hbar\alpha/F; 0) \\ &= \hat{U}(t + \hbar\alpha/F, 0; 2\pi/(Na))e^{i2\pi\hat{n}/N}\hat{U}(\tau, 0; 0)\hat{U}(0, t + \hbar\alpha/F; 0) \\ &= \hat{U}(t + \hbar\alpha/F, 0; 0)\bar{U}(0; 0)\hat{U}^{\dagger}(t + \hbar\alpha/F, 0; 0) \end{aligned} \tag{2.11}$$

In other words, $\bar{U}(t;\alpha)$ is unitarily similar to $\bar{U}(0;0)$, and therefore has a set of eigenvalues independent of both t and α.

We now claim that the characteristic frequencies of the system are of the form

$$\{\omega_j + 2\pi n_j/\tau, \quad n_j = \text{integers}, \ j = 1, 2, \ldots, N\}, \tag{2.12}$$

where $\{e^{-i\omega_j\tau}\}$ are the eigenvalues of $\bar{U}$, and it is understood that ω_j is defined modulo $2\pi/\tau$. To show this, we make an expansion,

$$g_0(n,t_0;\alpha) = \sum_j a_j(t_0;\alpha)u_j(n,t_0;\alpha), \tag{2.13}$$

where $u_j(n,t_0;\alpha)$ is the jth eigenstate of $\bar{U}(t_0;\alpha)$. Then equation (2.6) yields

$$g_l(n,t_0;\alpha) = \sum_j a_j(t_0;\alpha)e^{-i\omega_j\tau l}u_j(n,t_0;\alpha) \tag{2.14}$$

In terms of the wave function ψ, this is

$$\psi(n,t_0+l\tau) = e^{-i2\pi nl/N}\sum_j a_j(t_0;\alpha)e^{-i\omega_j\tau l}u_j(n,t_0;\alpha) \tag{2.15}$$

The overall factor, $e^{-i2\pi nl/N}$, is a gauge factor, and will be canceled out in the expectation value of any physical observable. It is easy to see that this is true for an operator that is diagonal in n. To demonstrate that this is also true for one with off-diagonals, consider the probability current from site n to site $n+1$,

$$J_{n,n+1}(t) = \frac{R}{2i\hbar}[e^{iFat/\hbar}\psi^*(n,t)\psi(n+1,t) - e^{-iFat/\hbar}\psi(n,t)\psi^*(n+1,t)]. \tag{2.16}$$

When t is increased from t_0 to $t_0+l\tau$, the gauge factors of the ψ's in the above expression are cancelled by the factors produced by $e^{iFat/\hbar}$ and its conjugate. The phase factors containing the ω's are the only ones left which depend on the time shift $l\tau$. In fact, the physical and gauge invariant time-shifting operator should be

$$e^{i2\pi\hat{n}l/N}\hat{T}(l\tau) \tag{2.17}$$

instead of $\hat{T}(l\tau)$, where $\hat{T}(l\tau)$ makes a pure time shift of $l\tau$ on a state. Therefore, the possible frequencies of the system are indeed of the form in (2.12).

The actu[illegible] procedure for determining the eigen-frequencies is very simple. First, we determine [illegible]$(t,0;0)$ by

$$\begin{aligned} i\hbar\frac{\partial}{\partial t}\hat{U}(t,0;0) &= \hat{H}(t)\hat{U}(t,0;0) \\ \hat{U}(0,0;0) &= \mathbf{1}\ , \end{aligned} \tag{2.18}$$

where the boundary condition (2.2) with $\alpha = 0$ is used. The matrix $e^{i2\pi\hat{n}/N}\hat{U}(\tau,0;0)$ is just $\bar{U}(t;\alpha)$ with zero t and α. The eigen-frequencies, being independent of t and α, are then obtained by diagonalizing $\bar{U}(0;0)$. Here, we would like to point out that the above procedure may be carried out in any representation which is convenient.

The upper time limit, τ, of the time dependent problem (2.15) is usually small, being inversely proportional to the system size N. Therefore, $\hat{U}(\tau,0)$ can be solved with ease and high precision. When N is very large, $\hat{U}(\tau,0)$ can be obtained perturbatively. To first order in τ, we have

$$\begin{aligned}\hat{U}(\tau,0) &\approx \exp[-(i/\hbar)\int_0^\tau dt\,\hat{H}(t)] \\ &\approx \exp[-(i\tau/\hbar)\hat{H}(0)].\end{aligned} \tag{2.19}$$

In this limit we have from (2.7) that

$$\bar{U}(0;0) \approx \exp\{\frac{\tau}{i\hbar}[\hat{H}(0) - Fa\hat{n}]\}. \tag{2.20}$$

Thus, the eigen-frequencies of $\bar{U}$ are closely related to the eigenenergies of $[\hat{H}(0) - Fa\hat{n}]$, the Hamiltonian in the static representation of the field. Our approach offers the convenience of eliminating the boundary effects for systems of finite size.

The eigenstates of $\bar{U}(t;\alpha)$ can also be easily found. We first look for the eigenstates, $\{u_j\}$, of $\bar{U}(0;0)$. Then, according to the last equality of equations (2.11), the eigenstates of $\bar{U}(t;\alpha)$ can be chosen as

$$e^{i\alpha a\hat{n}}\hat{U}(t + \hbar\alpha/F, 0; 0)\,u_j\,. \tag{2.21}$$

Before we close this section we would like to make two remarks. First, the dynamical symmetry presented above should be applicable to more general systems in any dimension than our one dimensional tight binding model. This fact follows from the generality of the symmetry of electric translations.

Secondly, all the results will remain valid, if the boundary condition (2.2) is replaced

by a fixed end type:

$$\psi(0,t) = \psi(N+1,t) = 0 \tag{2.22}$$

Of course, the group of dynamical symmetry in this case can be extended due to the fact that if $\psi(n,t)$ is a solution of (2.3) and (2.22), then

$$g_l(n,t) = e^{iFa\tau ln/\hbar}\psi(n,t+l\tau), \quad l = \text{integers} \tag{2.23}$$

are also solutions, with τ arbitrary. This is another way of saying that the time dependence of the Hamiltonian can be gauged away without changing the boundary condition (2.23). Such a transformation is not possible with the periodic boundary condition (2.2), so we had to make the restriction $\tau = h/FaN$ in (2.4).

3. Periodic potential and WS ladders

In this section, we consider the case of a periodic potential and examine the consequences of the symmetry of spatial translation on the frequency spectrum of the system.

If the potential in equation (2.3) satisfies

$$V_{n+p} = V_n \tag{3.1}$$

and the system size N is an integral multiple of the period p, then we can impose the Bloch condition on the states as

$$\psi(n+p,t) = e^{ikap}\psi(n,t) \tag{3.2}$$

where $0 \leq k < 2\pi/pa$, and k is discretized into N/p possible values according to the boundary condition (2.2). With the Bloch condition in place of (2.2), the Schrodinger equation (2.3) needs to be solved only for n in a period, say $1 \leq n \leq p$. The arguments and results presented in the last section can then be transcribed to here with the replacements: $N \to p$ and $\alpha \to k$.

Therefore, if $\hat{U}(t,t';k)$ is the evolution operator of equation (2.3) with the condition (3.2), then the unitary operator,

$$\bar{U}(t;k) \equiv e^{i2\pi\hat{n}/p}\hat{U}(t+T,t;k), \tag{3.3}$$

will have p eigenvalues of the form $\{e^{-i\omega_j T}\}$, with the ω's independent of t and k, where $T = h/Fap$. Moreover, if $\psi(n,t;k)$ is a solution of (2.3) and (3.2), then

$$\psi(n,t+T;k) = e^{-i2\pi n/p}\sum_{n'}\bar{U}_{nn'}(t;k)\psi(n',t;k). \tag{3.4}$$

The characteristic frequencies of the system then consist of p sequences:

$$\{\omega_j + 2\pi n_j/T, \quad n_j = \text{integers}, \ j = 1,2,...,p\}, \tag{3.5}$$

where it is understood that the ω's are defined modulo $2\pi/T$.

The average frequency spacing in the spectrum (3.5) is $Fa/\hbar$, the same as in (2.12), reflecting a conservation of level density. The spatial periodicity of the system has imposed a structure in the spectrum (2.12), that is, a periodicity over every group of p levels. In other words, the spectrum has been organized into p sets of levels, with a uniform spacing, $Fap/\hbar$, within each set. These correspond exactly to the WS ladders found before in various ways. In this sense, we say that the system is characterized by p sets of WS ladders, each represented by a ω_j.

To get some insights into the behavior of the states, we now go to a representation with the eigenstates of $\bar{U}$ as a basis. Consider the following expansion of an arbitrary state:

$$\psi(n,t) = \sum_k\sum_j C_j(t;k)u_j(n,t;k), \tag{3.6}$$

where $u_j(n,t;k)$ is an eigenstate of $\bar{U}(t;k)$ and satisfies the Bloch condition (3.2). The wave function inside the first summation symbol in the above expression should be a solution

of (2.3) and (3.2), and therefore is connected to its time translation as in (3.4). Then it follows that

$$\psi(n, t + lT) = e^{-i2\pi nl/p} \sum_{j,k} C_j(t; k) e^{-i\omega_j lT} u_j(n, t; k). \tag{3.7}$$

We will now see how the time evolution of the state is influenced by the fact that the ω's are independent of k. It will be convenient to consider, for a sequence of time $\{t_0 + lT,\ l = \text{integers}\}$, the density matrix defined by

$$\rho(n, n'; t_0 + lT) \equiv e^{i2\pi nl/T} \psi(n, t_0 + lT) \psi^*(n', t_0 + lT) e^{-i2\pi n'l/p}, \tag{3.8}$$

where the gauge invariant form of the time shifting operation has been used. (See equation (2.17) and the arguments given just above and below it for an explanation of this usage). Then it can be seen that the partial trace of the density matrix over j,

$$\sum_j \rho_{jj}(k, k'; t_0 + lT) = \sum_j C_j(t_0; k) C_j^*(t_0; k') \tag{3.9}$$

is independent of the time shifting, lT, where by definition

$$\rho_{jj'}(k, k'; t_0 + lT) = \frac{p}{N} \sum_{nn'} u_j^*(n, t_0; k) \rho(n, n'; t_0 + lT) u_{j'}(n', t_0; k'), \tag{3.10}$$

with $\{u_j(n, t_0; k)\}$ normalized over an unit cell. This means that the expectation value of any physical operator acting on k only is periodic in time. One trivial example of such an operator is the crystal momentum, k, itself. A more interesting one is the projection operator into a set of Wannier functions associated with the Bloch functions, $\{u_j(n, t_0; k)\}$, at the initial time t_0.[18] More specifically, the Wannier functions here are defined as

$$w_j(n - n_\mu; t_0) = \sqrt{\frac{p}{N}} \sum_k e^{-ikan_\mu} u_j(n, t_0; k), \tag{3.11}$$

where n_μ labels the position of the unit cells and can be taken for its value as 0, $\pm p$, $\pm 2p$, ..., etc. The arguments following (3.10) then indicate that the subspace spanned by $\{w_j(n - n_\mu; t_0);\ j = 1, .., p\}$ for a given n_μ is an invariant space of the system under time translations

by lT. In the case of $p = 1$, we can choose e^{ikan} as the eigenstate of $\bar{U}(t_0; k)$, which implies that the Wannier function will be strictly localized on a site. Therefore, a state initially localized on a site will again be localized on that site after a period of time $T = h/(Fa)$.

We now examine the localization property of the Wannier functions. The results of last section (especially (2.11) and (2.21)) indicate that, if $u_j(n, 0; 0)$ is the jth eigenstate of $\bar{U}(0; 0)$, then we can choose

$$u_j(n, t; k) = e^{i\omega_j \hbar k/F} e^{ikan} \sum_{n'} \hat{U}_{nn'}(t_0 + \hbar k/F, 0; 0)\, u_j(n', 0; 0) \tag{3.12}$$

as the jth eigenstate of $\bar{U}(t_0; k)$, where the summation is restricted on a unit cell. The n-independent phase factor, $e^{i\omega_j \hbar k/F}$, ensures the periodicity as k is increased by a reciprocal lattice number, $2\pi/(pa)$, as can be verified directly by using the general properties of $\hat{U}$ and $\bar{U}$ listed in (2.7) through (2.11) in the last section. From the theory of initial value problems of differential equations, $\hat{U}_{nn'}(t_0 + \hbar k/F, 0; 0)$ is an entire function of its time variable, and therefore of k. To summarize, $u_j(n, t; k)$ can be chosen such that it is a periodic and entire function of k, and that it satisfies the Bloch condition (3.2). All these properties ensure that the Wannier functions in (3.11) be localized, and that $w_j(n - n_\mu; t_0)$ go to zero faster than any exponential function as $|n - n_\mu|$ gets large.[19] The result of the last paragraph then tells us that, if a state is initially localized then it remains so in time.

4. Weak and strong field limits and model studies

In the weak field limit, the Hamiltonian in (2.3) varies slowly in time, and it can be useful to go to a representation with the adiabatic eigenstates of the Hamiltonian as a basis. Consider the expansion of an arbitrary state:

$$\psi(n, t) = \sum_{\beta, k} C_\beta(t; k) e^{ikan} \phi_\beta(n, k + Ft/\hbar) \tag{4.1}$$

where β is a band label, and $\phi_\beta(n,s)$, with $s = k + Ft/\hbar$, is an adiabatic eigenstate of the following problem

$$\begin{aligned} \epsilon_\beta(s)\phi_\beta(n,s) &= -R/2[e^{isa}\phi_\beta(n+1,s) + e^{-isa}\phi_\beta(n-1,s)] + V_n\phi_\beta(n,s) \\ \phi_\beta(n+p,s) &= \phi_\beta(n,s) \end{aligned} \tag{4.2}$$

It is seen from the above equation that the wave function,

$$e^{isan}\phi_\beta(n,s), \tag{4.3}$$

is just a Bloch function, with wave number s and energy $\epsilon_\beta(s)$, of the Hamiltonian in (2.3) in the absence of the electric field. It is well known that, if the Bloch bands do not cross one another, then the Bloch function can be chosen as a smooth and periodic function of the wave number.[19] Therefore, we can impose the additional condition on ϕ as

$$\phi_\beta(n, s + 2\pi/pa) = e^{-i2\pi n/p}\phi_\beta(n,s). \tag{4.4}$$

Now, the following wave function,

$$\sum_\beta C_\beta(t;k)e^{ikan}\phi_\beta(n, k + Ft/\hbar), \tag{4.5}$$

in the expansion (4.1) should satisfy (2.3) and (3.2), so it is connected to itself a period T time later by $\bar{U}(t;k)$ as in (3.4). It then follows that

$$C_\beta(t+T;k) = \sum_{\beta'} \tilde{U}_{\beta\beta'}(t;k)C_{\beta'}(t;k), \tag{4.6}$$

where

$$\tilde{U}_{\beta\beta'}(t;k) = \sum_{nn'} e^{ika(n'-n)}\phi^*_\beta(n, k + Ft/\hbar)\phi_{\beta'}(n', k + Ft/\hbar)\bar{U}_{nn'}(t;k), \tag{4.7}$$

assuming that the ϕ's are normalized in the unit cell. Thus, $\tilde{U}$ is unitarily similar to $\bar{U}$ and must have the same set of eigenvalues.

The equation of motion for the expansion coefficients, C_β, can be found by substituting (4.1) and (4.2) into (2.3), with the results

$$i\hbar\frac{\partial}{\partial t}C_\beta(t;k) = \epsilon_\beta(k+Ft/\hbar)C_\beta(t;k) + \sum_{\beta'} X_{\beta\beta'}(k+Ft/\hbar)C_{\beta'}(t;k), \tag{4.8}$$

where the inter-band coupling matrix, $X(s)$, is given by

$$X_{\beta\beta'}(s) = F\sum_n \phi^*_\beta(n,s)i\frac{\partial}{\partial s}\phi_{\beta'}(n,s) \tag{4.9}$$

So far, the results have been exact so long as the bands do not cross one another. The adiabatic approximation amounts to dropping the off-diagonal elements of $X(s)$. Then, equation (4.8) can be easily solved to yield

$$C_\beta(t+T;k) = C_\beta(t;k)\exp\{\frac{-i}{\hbar}\int_0^T [\epsilon_\beta(k+Ft/\hbar) + X_{\beta\beta}(k+Ft/\hbar)]\}, \tag{4.10}$$

with the evolution operator $\tilde{U}(t;k)$ diagonal in the band index, and with the eigenfrequencies given by

$$\hbar\omega_\beta = < \epsilon_\beta > + < X_{\beta\beta} >, \tag{4.11}$$

where the angular brackets denote averages over a period of time, T. That the eigenfrequencies are independent of t and k can be seen from the fact that both ϵ_β and $X_{\beta\beta'}$ depend on t and k through the combined variable $(k+Ft/\hbar)$ and are periodic in time with period T.

The formula (4.11) says that $\hbar\omega_\beta$ is equal to the average band energy plus an extra term $< X_{\beta\beta} >$. The extra term is in general nonzero, and can be related to the Berry phase associated with the adiabatic eigenvalue problem (4.2). If we had imposed on ϕ the condition of parallel transport,

$$\sum_n \phi^*_\beta(n,s)\frac{\partial}{\partial s}\phi_\beta(n,s) = 0, \tag{4.12}$$

then there would have been an extra phase factor $e^{-i\Gamma_\beta}$ multiplying the right hand side of (4.4). The phase Γ_β is called the Berry phase for the β's adiabatic level of (4.2), with its value given by

$$\Gamma_\beta = \frac{2\pi}{Fap} < X_{\beta\beta} >, \tag{4.13}$$

where $< X_{\beta\beta} >$ should be evaluated with the original condition (4.4).[17] Since the Berry phase is independent of the field, the term $< X_{\beta\beta} >$ is proportional to the field. It is seen that (4.11) is really the first two terms in an expansion in powers of the field strength.

The correction to the adiabatic approximation (4.10) will be exponentially small when $X_{\beta\beta'}/(\epsilon_\beta - \epsilon_{\beta'})$, for $\beta \neq \beta'$, is small. Since $X_{\beta\beta'}$ is of order $Fap/(2\pi)$, the criterion for a good approximation is

$$Fap/(2\pi\Delta_{\beta\beta'}) \ll 1, \tag{4.14}$$

where $\Delta_{\beta\beta'}$ is the minimum gap between the βth and β'th energy bands.[4] The corrections will in general show up in the off-diagonal elements of $\tilde{U}$, and lift the degeneracies (if any) in the adiabatic eigenvalues $\{e^{-i\omega_\beta T}\}$. This fact has also been noticed by other authors.[9]

Now consider the strong field limit. We can then make a first order time-dependent approximation for the unitary matrix $\hat{U}(T,0;0)$, because the time period $T = h/(Fap)$ will be small. Therefore

$$\begin{aligned} \hat{U}(T,0;0) &\approx \exp[\frac{-i}{\hbar}\int_0^T \hat{H}(t)\,dt] \\ &= \exp[(-iT/\hbar)\bar{H}], \end{aligned} \tag{4.15}$$

where

$$\bar{H}\psi(n) = -\frac{R}{2}\frac{p}{\pi}\sin(\pi/p)[e^{i\pi/p}\psi(n+1) + e^{-i\pi/p}\psi(n-1)] + V_n\psi(n). \tag{4.16}$$

The corresponding approximation for $\bar{U}(0;0)$ is then

$$\hat{U}_{nn'}(0;0) \approx e^{-i2\pi n/p}\sum_{m=1}^{p}\phi_m(n)\phi_m^*(n')e^{-iT\epsilon_m/\hbar}, \tag{4.17}$$

where $\{\epsilon_m, \phi_m(n)\}$ are the eigenenergies and eigenstates (orthonormalized over a unit cell) of (4.16). When $T \to 0$, the matrix (4.17) will be diagonal in n, due to the completeness of the eigenstates $\{\phi_m(n)\}$. The p diagonal elements $e^{-i2\pi n/p}$ are all different, so when the off-diagonals are small compared with the minimum level distance, $2\sin(\pi/p)$, the eigenvalues of $\bar{U}(0;0)$ can be approximated by

$$\exp[-i(2\pi n/p + T\bar{\epsilon}(n)/\hbar)] \tag{4.18}$$

where

$$\bar{\epsilon}(n) = \sum_m \epsilon_m \phi_m(n)\phi_m^*(n) \tag{4.19}$$

is the average energy on the site n. In view of the above arguments, the condition for the strong field approximation should be

$$\frac{T}{\hbar} R \frac{p}{\pi} \ll 1. \tag{4.20}$$

We will now study a concrete model to illustrate the ideas presented above and in the previous sections. Specifically, we take the site potential in the form

$$V_n = V\cos(\frac{2\pi q}{p}n), \tag{4.21}$$

where q and p are mutually inconmmensurate integers so that p is the fundamental period of the potential. Without the electric field, the Schrodinger equation (2.3) with this potential is the time dependent form of the well known Harper's equation or the discrete Mathieu's equation.[20] Harper's equation has been extensively studied in the context of two dimensional periodic systems in a uniform magnetic field. Our study here will be applicable to such systems with an additional electric field applied on them.[21] What we like to know particularly is how the eigen-frequencies behave when the field or other parameters are varied.

The case of $p = 1$ is very simple. The solution of (2.3) and (3.2) can be found exactly as

$$\psi_k(n,t) = e^{ikan} \exp[\frac{1}{i\hbar} \int_0^t dt' \, (-R\cos(Fat'/\hbar + ka) + V)]. \tag{4.22}$$

This is the so called Houston function for the Bloch band under consideration. The unitary operator $\bar{U}$ is now a scalar and can be read off from the above as

$$\begin{aligned} \bar{U} &= \exp[\frac{1}{i\hbar} \int_0^{h/(Fa)} dt' \, (-R\cos(Fat'/\hbar + ka) + V)] \\ &= e^{-i2\pi V/Fa}, \end{aligned} \tag{4.23}$$

with $\omega = V/\hbar$, which is independent of k as expected. The single set of WS ladders is then

$$\{\omega + nFa/\hbar, \quad n = \text{integers}\}. \tag{4.24}$$

We expect that these uniformly spaced levels will, in general, be modulated to non-uniform ones in the presence of a varying potential; the modulation will be periodic if the potential is periodic.

When $p > 1$, exact solutions are hard to find, and numerical calculation has to be invoked. We have considered several cases, each to reveal one or more aspects of the behavior of the eigen-frequencies. In the figures (1a-1e) presented and analyzed below, the reduced eigen-frequencies $\{\hbar\omega_j/(Fa), \; j = 1, ..., p\}$ are plotted against $R/(Fap)$, namely the inverse field scaled by the hopping amplitude, R. Since $\omega_j T = \omega_j h/(Fap)$ is only defined modulo 2π, we found it convenient to fold $\hbar\omega_j/(Fa)$ inside the range $[0.5, p + 0.5)$. The reader should be aware, however, that the whole frequency spectrum extends periodically both upwards and downwards. The other dimensionless parameter besides $R/(Fap)$ is V/R. We have taken it as 0.5 for the first three figures and 0.1 for the last two in order to study the limit of small band splittings.

Figure 1a corresponds to $q/p = 1/2$. In the strong field limit, the spacing between the two ω's approaches $Fa/\hbar$, meaning that the whole spectrum reduces to the single set of

WS ladders (4.24) of the parent band. The initial slopes of the two levels agree perfectly well with the prediction of (4.18), which now has the form:

$$\begin{aligned} \hbar\omega_1/(Fa) &= 1 - 2V/(Fap) \\ \hbar\omega_2/(Fa) &= 2 + 2V/(Fap). \end{aligned} \tag{4.25}$$

Deviation from the above behavior becomes pronounced when $R/(Fap) > 0.2$. As the field gets weaker, the levels approach straight lines with decreasingly small repulsions at their intersections. The straight line behavior is a manifestation of the adiabatic limit. (The band structure of (4.2) is shown in figure 2a.) The expression (4.11) can be evaluated with little effort to give

$$\begin{aligned} \hbar\omega_1/(Fa) &= g(R/Fap) \\ \hbar\omega_2/(Fa) &= 1 - g(R/Fap), \end{aligned} \tag{4.26}$$

where

$$g = 2\int_0^1 ds\,\sqrt{(V/R)^2 + \cos^2(\pi s)}, \tag{4.27}$$

with $g = 1.67761$ at $V/R = 0.5$. When the expressions in (4.26) are folded in the range of the plot, they match very well with the levels in the figure for $R/(Fap) > 1$. The level repulsions at their intersections are due to the coupling of the two adiabatic bands. The size of the gaps generated by level repulsions decreases exponentially with decreasing field, that is,

$$\delta(\hbar\omega/(Fa)) \sim \exp(-\lambda R/(Fap)), \tag{4.28}$$

where the exponent λ is about 0.77 for $V/R = 0.5$.

Figure 1b is for $q/p = 1/4$. The new feature appeared in this case is that two of the levels are horizontal lines. Explicit calculation shows that the four adiabatic bands are symmetrically located about $\epsilon = 0$, and that the central two are degenerate (see figure 2b). If we treat the degenerate bands as one big band and apply the adiabatic approximation to it, then we obtain the two horizontal levels in the figure. They are horizontal, because the average energy of the combined band is zero. The Berry phase term never gives rise to a nonzero slope in our plot, and it only shifts the levels vertically to their right positions.

Figure 1c corresponds to the case of $q/p = 2/5$. As noted before, the levels at weaker fields approach those of the adiabatic approximation, with steeper lines corresponding to bands farther away from the zero energy. (See figure 2c for the band structure.) The adiabatic level corresponding to the central band should be nearly a horizontal line at about 2.5 vertically, but is interrupted into segments due to the repulsion with the other adiabatic levels. On the other hand, the initial positions and slopes of the levels in the strong field limit are well accounted for by the approximation (4.18).

In the zero potential limit, the levels should become those of the WS ladders of the parent Bloch band, that is, they should become horizontal lines with integral heights in our plot. To study the effect of a weak periodic potential, let us consider again the cases $q/p = 1/2$ and $2/5$, but with $V/R = 0.1$. The results are displayed in figures 1d and 1e. It is seen that the levels are modulated up and down sinusoidally about the WS ladders of the parent band, as the field strength is varied. The amplitude of modulation increases with decreasing field, while the frequency of modulation approaches to a constant. A quantitative analysis of these results will be given in the next section.

5. Floquet theorem and weak potential limit

In this section we will make use of the symmetry associated with the explicit time-periodicity of the Schrodinger equation (2.3) by applying the Floquet theorem.[22] As one will see below, this approach will lead to a very compact theory for the WS ladders of the parent Bloch band under weak perturbation.

The theorem tells us that the evolution operator of equation (2.3) can be written in the form

$$\hat{U}(t,t') = e^{-iW(t-t')}Z(t,t'), \tag{5.1}$$

where W is Hermitian and independent of time, and $Z(t,t')$ is unitary and periodic in t and t' with period $h/(Fa)$. The time evolution of the system is then characterized by a set of frequencies given by the eigenvalues of W plus integral multiples of $Fa/\hbar$. Because of its additive multiplicity, the frequency spectrum can also be determined by the eigenvalues of the following operator

$$e^{-iWh/(Fa)} = \hat{U}(h/(Fa),0) \equiv \bar{U}, \tag{5.2}$$

where the first equality comes from the periodicity of Z and from the fact that $Z(0,0)$ is the *unity* operator. By definition, $\bar{U}$ is just the evolution operator over the first period. The above relation indicates that, if $\{e^{-i\omega_m h/(Fa)}\}$ is the set of eigenvalues of $\bar{U}$, then the frequency spectrum is given by $\{\omega_m\}$ plus integral multiples of $Fa/\hbar$.

The operator $\bar{U}$ here also has a simple relationship with those introduced in the previous sections in the same notation. It is, in fact, equal to the Nth power of that in section 2, and the pth power of that in sections 3 and 4. As a result, the frequency spectrum given in this section will correspond to those modulo $Fa/\hbar$ in the previous sections. It will be helpful to notice that we have been looking at the problem (2.3) in three different time scales: $h/(FaN)$ in section 2, h/Fap in sections 3 and 4, and h/Fa here in this section. The degeneracy of the frequency spectrum when viewed from a longer time scale should correspond to a periodic structure of the spectrum viewed from a shorter time scale, and vice versa.

When the potential V_n is weak and the field is strong, we can make a first order perturbation approximation for $\bar{U}$. It is convenient to expand

$$\psi(n,t) = \sum_k a(k,t) e^{ikan} \exp[\frac{iR}{\hbar}\int_0^t dt' \cos(Fat'/\hbar + ka)], \tag{5.3}$$

where the momentum k takes the same set of values as in (3.2). Substituting this into the

Schrodinger equation (2.3) then yields

$$i\hbar\frac{\partial}{\partial t}a(k,t) = \sum_{k'} a(k',t)\,V(k-k')\exp\{\frac{iR}{\hbar}\int_0^t dt'[\cos(Fat'/\hbar + k'a) - \cos(Fat'/\hbar + ka)]\}, \tag{5.4}$$

where

$$V(k-k') = \frac{1}{N}\sum_n e^{-i(k-k')an}\,V_n \tag{5.5}$$

To first order in the potential, we have

$$\begin{aligned} a(k,h/(Fa)) &= a(k,0) \\ &+ \frac{2\pi}{iFa}\sum_{k'} a(k',0)V(k-k')e^{\frac{iR}{Fa}[\sin(ka)-\sin(k'a)]}J_0(\sin((k-k')a/2)2R/(Fa)), \end{aligned} \tag{5.6}$$

where $J_0(x)$ is the zeroth order Bessel function. Now, if we make a further expansion,

$$a(k,t) = e^{\frac{iR}{Fa}\sin(ka)}\sum_m e^{-ikam}b(m,t), \tag{5.7}$$

where m takes integer values $1,2,..,N$, then

$$b(m,h/(Fa)) = b(m,0)\{1 + \frac{2\pi}{iFa}\sum_k V(k)e^{ikam}J_0(\sin(ka/2)2R/(Fa))\} \tag{5.8}$$

Therefore, $\bar{U}$ is diagonalized to first order in V by the transformations (5.3) and (5.7), with the eigen-frequencies given by

$$\hbar\omega_m = \sum_k V(k)e^{ikam}J_0(\sin(ka/2)2R/(Fa)). \tag{5.9}$$

This expression can also be written in terms of V_n as

$$\hbar\omega_m = \sum_n V_n\int_0^1 ds\,J_{2(n-m)}(\cos(2\pi s)2R/(Fa)), \tag{5.10}$$

where we have taken the limit $N \to \infty$.

When the potential is zero (or constant), the eigenvalues of $\bar{U}$ are all degenerate, implying that any state is an eigenstate of $\bar{U}$. Therefore, the approximation described in the last paragraph is really that of a first order degenerate perturbation. It can be seen

from (5.9) or (5.10) that the degeneracy is lifted in first order by a general potential. The perturbed eigenstates can be found by tracing back the transformations (5.7) and (5.3) as

$$\begin{aligned} u_m(n) &= \frac{1}{N}\sum_k e^{\frac{iR}{Fa}\sin(ka)} e^{ika(n-m)} \\ &= \sum_l J_{m-n+lN}(R/(Fa)), \end{aligned} \tag{5.11}$$

where the last summation is over integers ensuring the boundary condition (2.2). In the limit of $N \to \infty$, we have

$$u_m(n) = J_{m-n}(R/(Fa)), \tag{5.12}$$

a much simpler result. It is noticed that the last expression is also the eigenstate of the Hamiltonian in (2.3) in the static representation of the electric field, with an uniform site potential and an infinite system size.

The formula (5.10) is very convenient when the effect of a few impurities is concerned. Consider, for instance, the case that V_n is zero everywhere except at the origin $n = 0$. Then we have

$$\hbar\omega_m = V_0 \int_0^1 ds\, J_{2m}(\cos(2\pi s) 2R/(Fa)). \tag{5.13}$$

In figure 3a, exact numerical results for $\{\hbar\omega_m/V_0\}$ are plotted against $R/(Fa)$, where we have taken $V_0/R = 0.1$. The above formula gives a very good account of the behavior of the levels. In the strong field limit, the levels are degenerate except for the one corresponding to $m = 0$ in the above formula. As the parameter $R/(Fa)$ is increased from zero, there are two levels peeled off from the degenerate center to second order in $R/(Fa)$, then another two to fourth order in $R/(Fa)$, and so on. This behavior of the levels can be understood from the localization property of the eigenstates (5.12): as the parameter $R/(Fa)$ is increased, the localization length of the states become longer, and therefore more and more sites feel the existence of the impurity. At weaker field strengths, the levels which are already outside the degenerate center begin to oscillate, accompanying the continuous peeling-off of new

levels from the center. In figure 3b, $\{\hbar\omega_m/(Fa)\}$ are plotted against $R/(Fa)$, where we have taken again $V_0/R = 0.1$.

For a periodic potential of the form (4.21), a very compact formula for the levels can be derived from (5.9) as

$$\hbar\omega_m = V\cos(\frac{2\pi q}{p}m)J_0(\sin(\pi q/p)2R/(Fa)). \tag{5.14}$$

Evidently, the levels bunch into p degenerate branches, which is a consequence of the periodicity of the potential, and is true even if the potential is strong. Remembering that the spectrum defined in this section corresponds to those modulo $Fa/\hbar$ in the previous sections, one can read off the degeneracy from the periodic structure of the spectrum in (5.3). The above formula has been tested numerically, and is shown to give a quantitatively good account of the oscillatory behavior of the levels in figures 1d and 1e.

The formula (5.14) shows a further coalesce of the p branches into one, for a infinite discrete set of values of the parameter $R/(Fa)$ where the Bessel function vanishes. This is, of course, generally true only to first order in the potential corresponding to the degree of our approximation. It can be shown, however, that for $p = 2$ the degeneracy occurs infinitely many times as the parameter $R/(Fa)$ is varied, even if the potential is strong. The degeneracy of the two branches corresponds to where the two levels $\{\hbar\omega_j/(Fa)\}$ in figures 1a and 1d have a distance of unity. When all the eigenvalues are the same, the evolution operator $\bar{U}$ is proportional to the unity operator, and therefore every initial state will evolve back to itself after a period of time, $h/(Fa)$. As has been seen many times in this section and the previous sections, this is the case for the unperturbed parent Bloch band. We now see the recurrence of the states at particular values of the parameter $R/(Fa)$, if the parent band is split into two. The formula (5.14) predicts an approximate recurrence of the states, when the potential is periodic and weak.

6. Conclusion and discussion

In this paper, the effect of a constant and uniform electric field on a split Bloch band is studied through a tight binding model. We have shown how the WS ladders of the parent band is modified by a splitting potential, and how the frequency spectrum behave as a function of the field strength sweeping from the weak to the strong limit. In the case that the parent band is split into a finite number of sub-bands, we have also established a new result concerning the time evolution of the system. Further, we have developed a theoretical framework, which exploits the symmetries of the system and allows for easy and clean numerical calculations.

The general analysis has been guided by the symmetry group of electric translations[14], namely the gauge covariant space-time translations, which exhibit the physical uniformity of the electric field. Three Abelian subgroups of the electric translations have been used, each emphasizing certain aspects of the system. The results obtained in different ways are related and complementary.

The first subgroup emphasizes the temporal uniformity of the system. The resultant dynamical symmetry described in section 2 enables us to characterize the time evolution by a set of eigen-frequencies, and offers us a general and convenient calculational framework for a system with or without a spatial symmetry. For large systems, the eigen-frequencies are the same as the eigenenergies (divided by $\hbar$) of the Hamiltonian in the static representation of the field. For finite systems, the approach offers the convenience of eliminating the boundary effect, if bulk properties are the basic concern. Yet, when necessary, one can always insert an infinite potential somewhere to effectively break the ring geometry into a simply connected one with fixed-end boundary conditions.

The second subgroup emphasizes the spatial translational symmetry that the system may have. An immediate consequence is the periodic structure of the frequency spectrum, revealing the WS ladders in a natural way. An important result has been obtained regarding the spatial and temporal behavior of the states in an isolated multi-band system.

There exists a set of subspaces to which the states return periodically in time; and the constituent states in each of the subspaces are localized (more than exponential) around a given unit cell. This result is a generalization of the periodic recurrence of the states derived from a single band approximation. Since a localized state returns after a finite time interval, the state can only travel a finite distance. In this sense we say that the states are localized.

The following problem has been studied in detail: how are different set of WS ladders are relatively placed in the frequency spectrum, and how do their positions depend on the field and other parameters? The study is guided by the analytic results obtained in the weak and strong field limits and in the weak potential limit. Exact numerical results for the frequency levels have been displayed for several cases of a model periodic potential. When the field is weak, the levels are shown to behave according to the prediction of the adiabatic (or single-band) approximation. The Berry phases are in general nonzero and shift the levels to their right positions. The interband couplings show up as level repulsions where the adiabatic frequency levels try to cross one another. The sizes of the gaps generated at the intersections depend exponentially on the field and are very small for weak field values. The gaps widen as the field gets strong, with the spectral structure smoothly transformed to that in the strong field limit. As expected from the analytical approximation appropriate for this limit, the levels become those of the parent band, individually shifted by the site energies, showing the extreme localization of the states. The initial slopes of the levels, as the inverse field deviates from zero, are also correctly predicted by the theory.

The explicit time periodicity of the Hamiltonian is exploited by the Floquet theorem. The appropriate subgroup of electric translations is the one with a basic time step equal to the period of Bloch oscillation of the parent band. Weak perturbation of the WS ladders of the parent band can be studied this way and a simple and general formula has been derived for the perturbed levels. For a weak periodic potential, the WS levels of the parent

band are shown to be modulated up and down sinusoidally as a function of the inverse field. The amplitudes of modulation increase as the field gets weak, while the frequency of modulation approaches a constant. Such behavior of the levels is closely described by a very compact formula. Another interesting phenomenon revealed is the approximate (to second order in the potential) recurrence of an arbitrary state, for an infinite set of values of the field or other parameters. The period of recurrence is that of Bloch oscillation of the parent band. For a two band system, the recurrence is expected to be exact. Finally, the effect of a single impurity has also been considered and analyzed in detail.

Having summarized our basic results, we now make a few remarks regarding the generality and limitation of our approach and the results. First, the notion of electric translations should be applicable to more general systems: one dimensional or higher dimensional, discrete or continuous. In this paper we have limited our attention to a system whose dynamics is invariant under continuous time translations. What can happen if the dynamics is invariant under discrete time translations only? Question of commensuration will arise if the dynamics also has a spatial periodicity. In this case, an Abelian subgroup of electric translations exists as a symmetry group, only when the product of temporal and spatial periods is a rational multiple of h/F. The situation is analogous to a two dimensional electron system in a periodic potential and a uniform magnetic field.

Secondly, most of our results will remain valid if our tight binding model is modified to a more general form: with hopping amplitudes nonzero beyond the nearest neighbors and/or dependent on positions, except for the requirement of short ranged inter-site couplings. For example, the conclusion about the existence of localized invariant subspaces will remain true, since it was drawn from a symmetry consideration and from a fact concerning a finite set of first order differential equations. Another example is the approximate recurrence of states when the parent band is weakly perturbed.

Thirdly, difficulties will arise, however, for a continuous system when all of the inter-

band couplings are taken into account. According to ref. 4, the spectrum will become continuous without any gaps. Therefore, the validity of the notion of WS ladders become doubtful. The problem does not bother us too much, if only a finite number of bands (or a finite spectral range) is concerned, and if these are bounded by large energy gaps. The defense is to invoke the usual wisdom concerning the weakness of Zener tunneling across big gaps, and to regard the results as valid for long, but not infinitely long, time scales.

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Bloch bands of the evolution operator, instead of the Hamiltonian in the absence of the electric field. For an elementary treatment of the Wannier functions, see Chap. 5 in Callaway's textbook listed in ref. 6.

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FIGURE CAPTIONS

Figure 1. Reduced frequency levels $\{\hbar\omega_j/(Fa), j = 1,..,p\}$ as functions of $R/(Fap)$ for the discrete cosine potential (4.21). (a) $q/p = 1/2$, $V/R = 0.5$; (b) $q/p = 1/4$, $V/R = 0.5$; (c) $q/p = 2/5$, $V/R = 0.5$; (d) $q/p = 1/2$, $V/R = 0.1$; (e) $q/p = 2/5$, $V/R = 0.1$. These levels repeat periodically both upwards and downwards in the frequency spectrum. As a reference, the levels for the parent band ($V = 0$) are horizontal lines at integral heights.

Figure 2. Band energies $\{\epsilon_\beta(s),\ \beta = 1,..,p\}$ for the adiabatic eigenvalue problem described in (4.2) in the text. The potential is $V_n = V\cos(2\pi q/p)$, with $V = 0.5$. The hopping amplitude is $R = 1$. The parameter q/p is (a) 1/2, (b) 1/4, and (c) 2/5 respectively.

Figure 3. Frequency levels as functions of $R/(Fa)$ for a single impurity potential, with $V_0/R = 0.1$. The levels have been folded into an interval $-0.5 < \hbar\omega/(Fa) \leq 0.5$, corresponding to a level spacing in the frequency spectrum of the parent band. (a) $\{\hbar\omega_m/V_0\}$ are plotted. Note the Bessel-function like behavior of the levels. (b) $\{\hbar\omega_m/(Fa)\}$ are plotted. Integral heights in this plot correspond to the levels of the parent band.

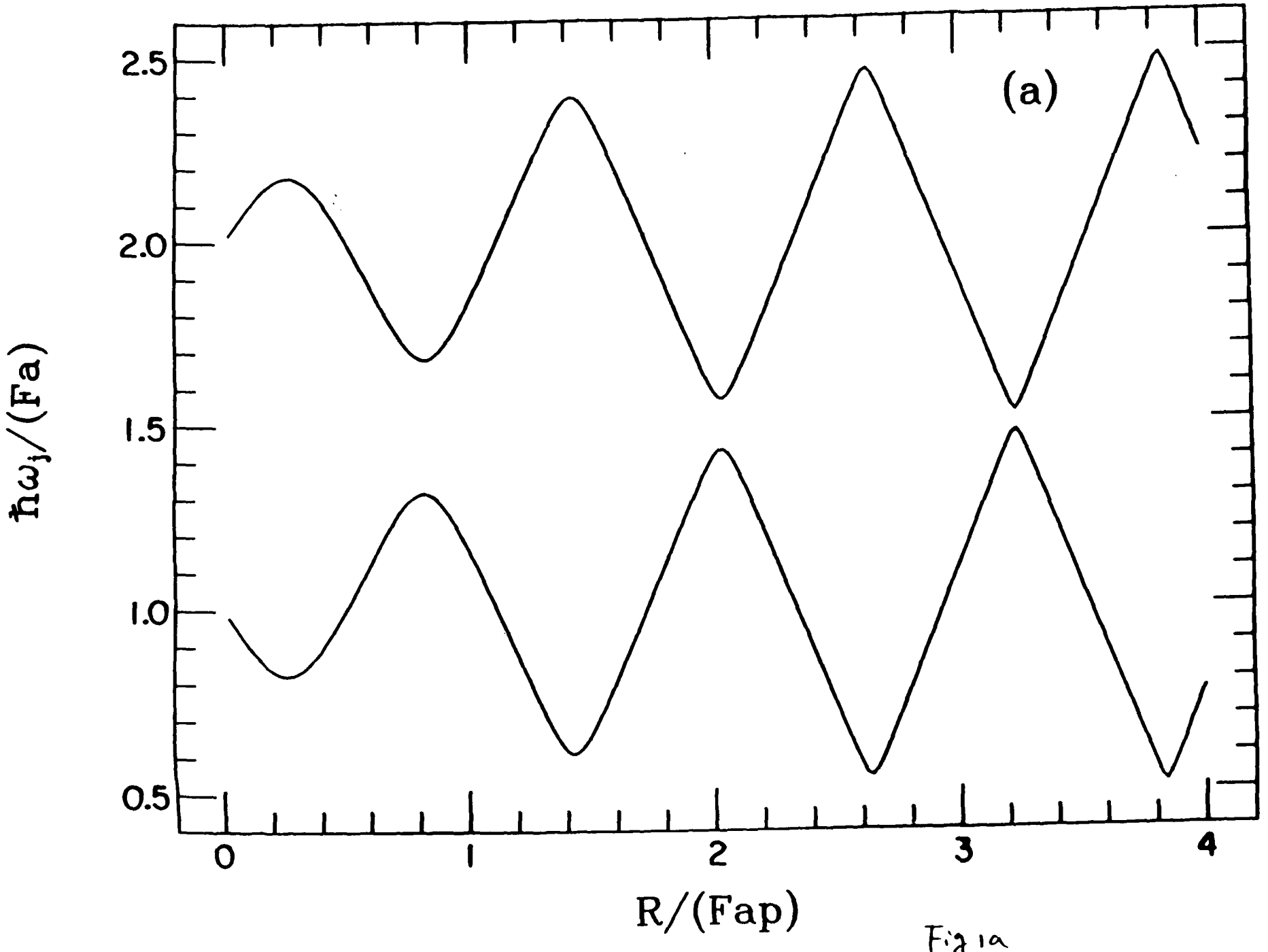


Fig 1a

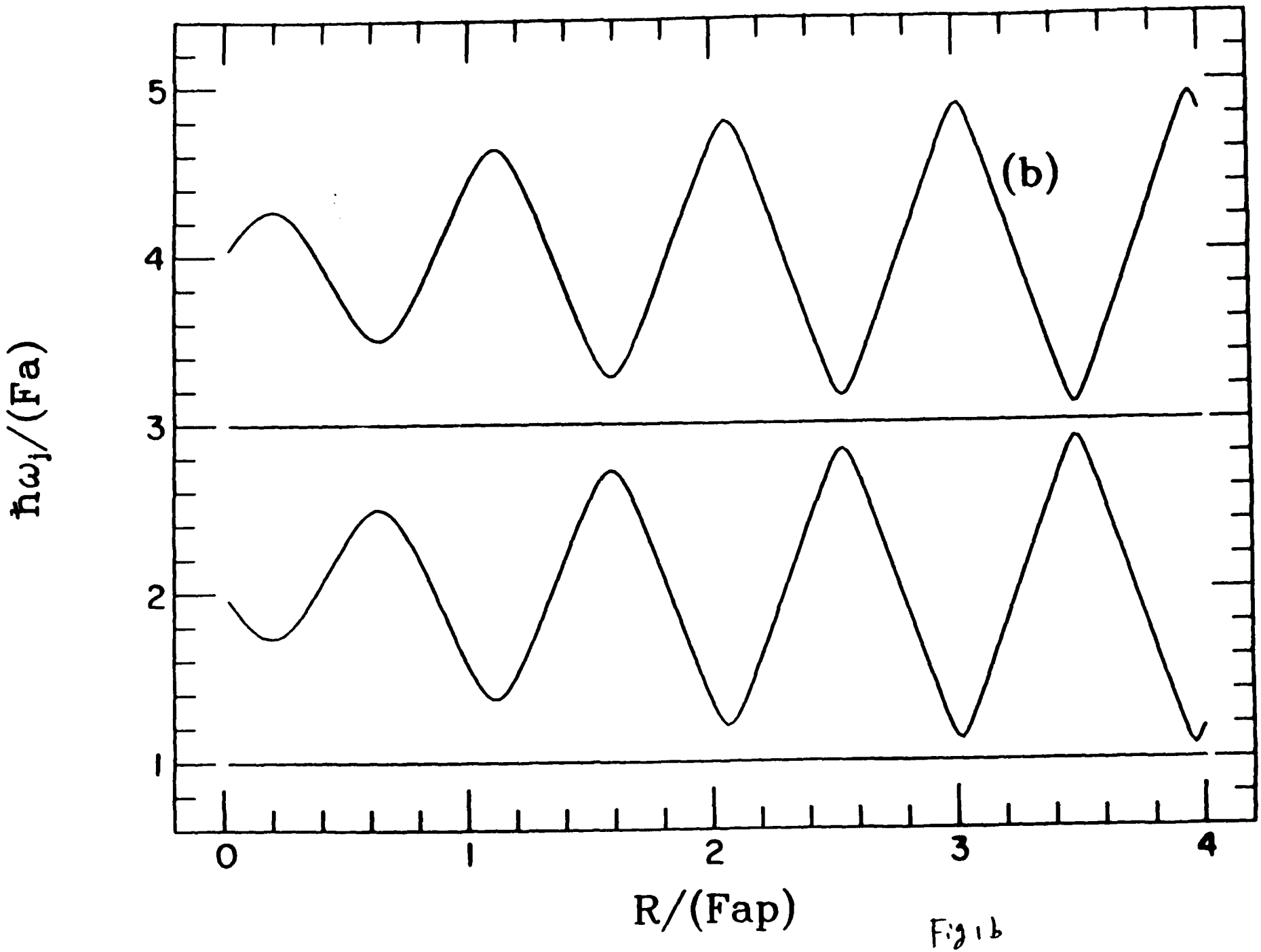


Fig 1b

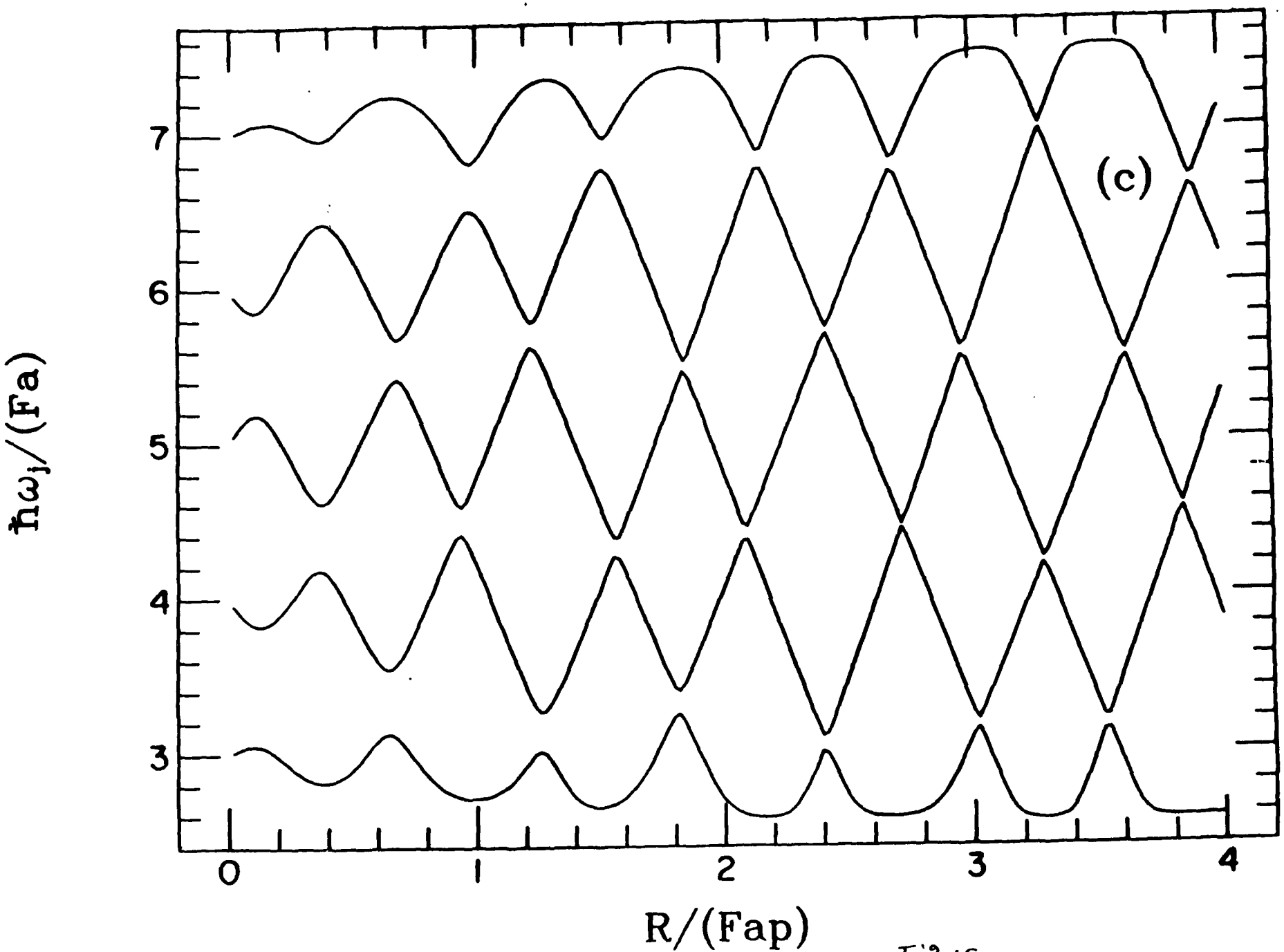
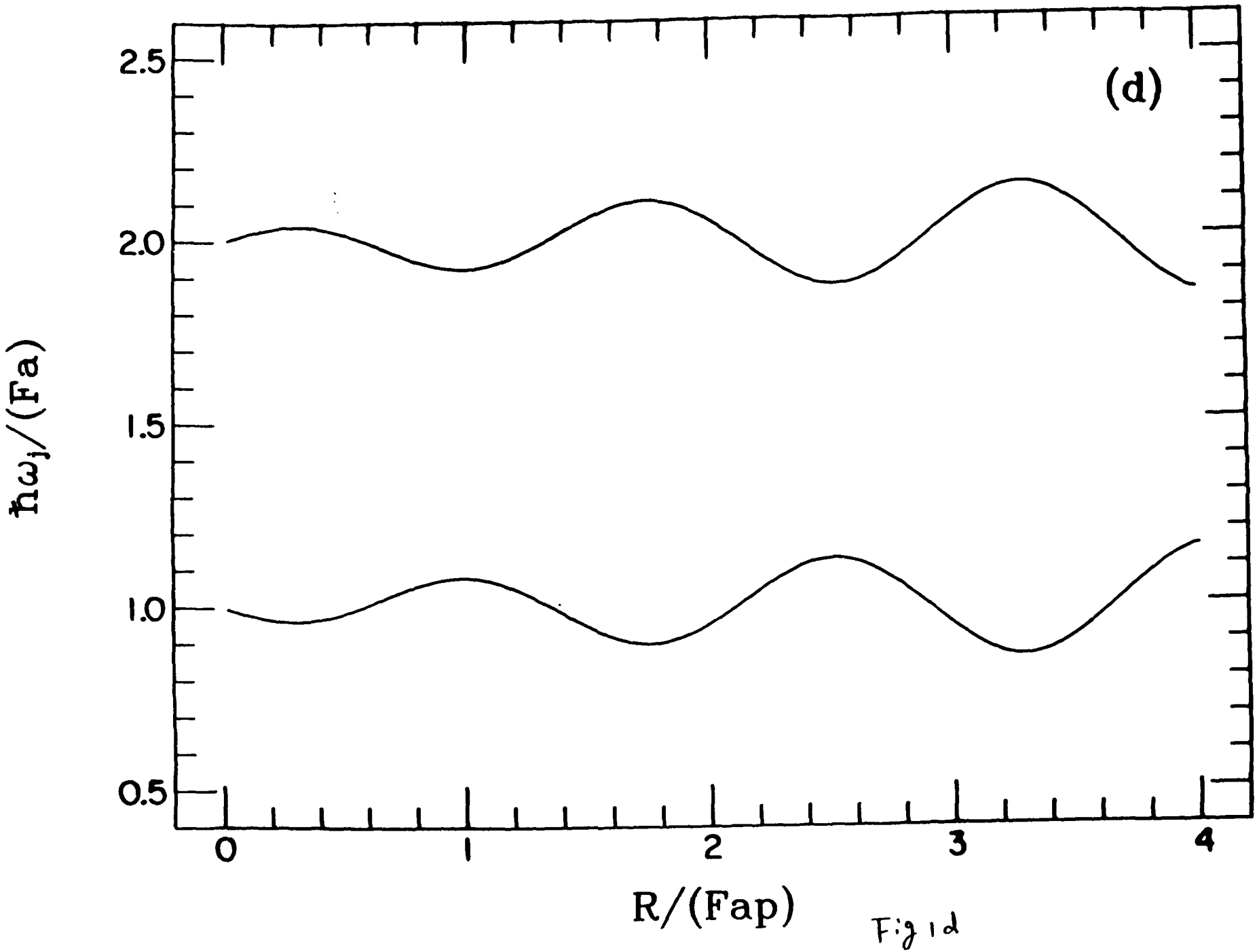


Fig 1c



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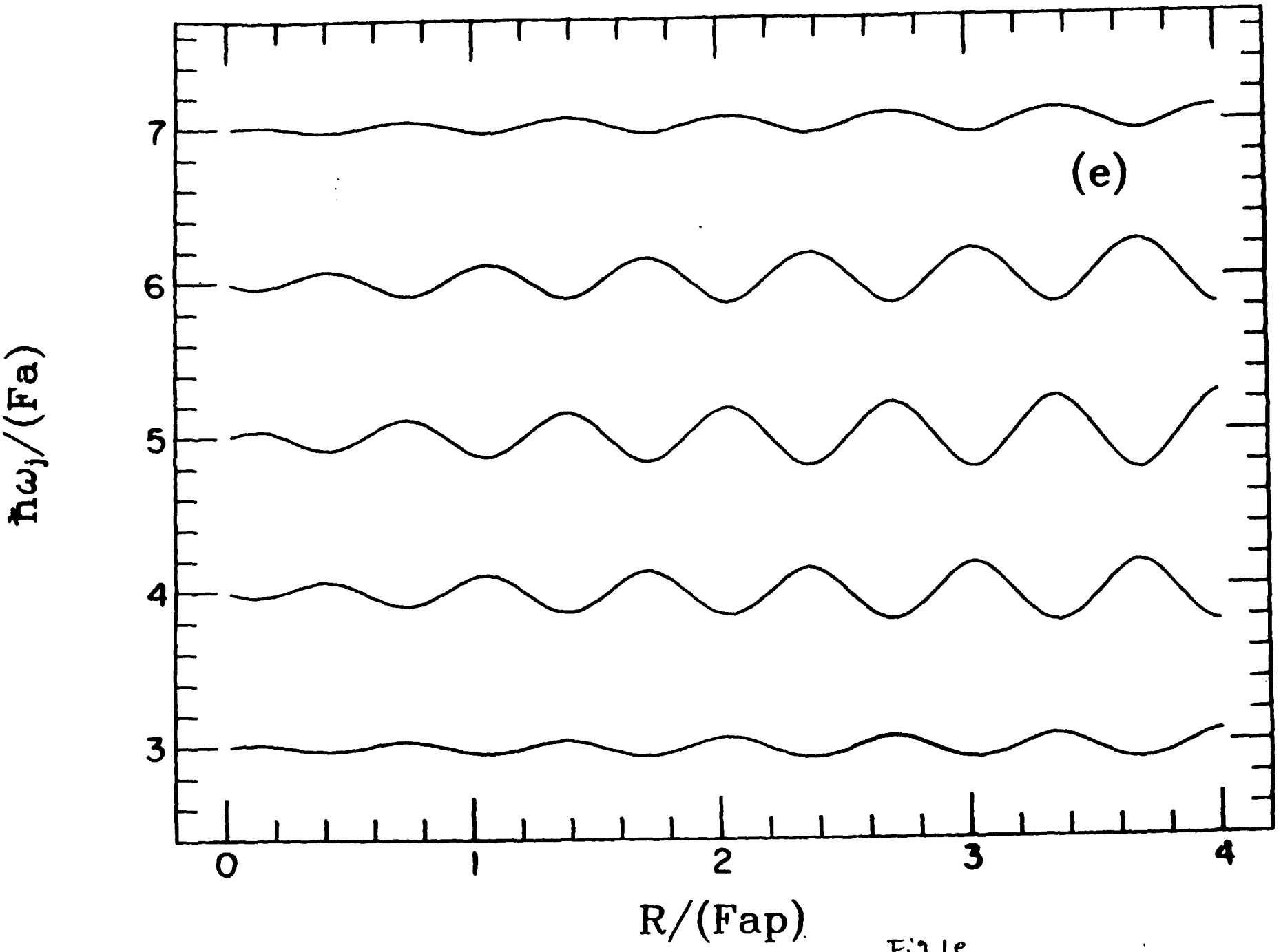

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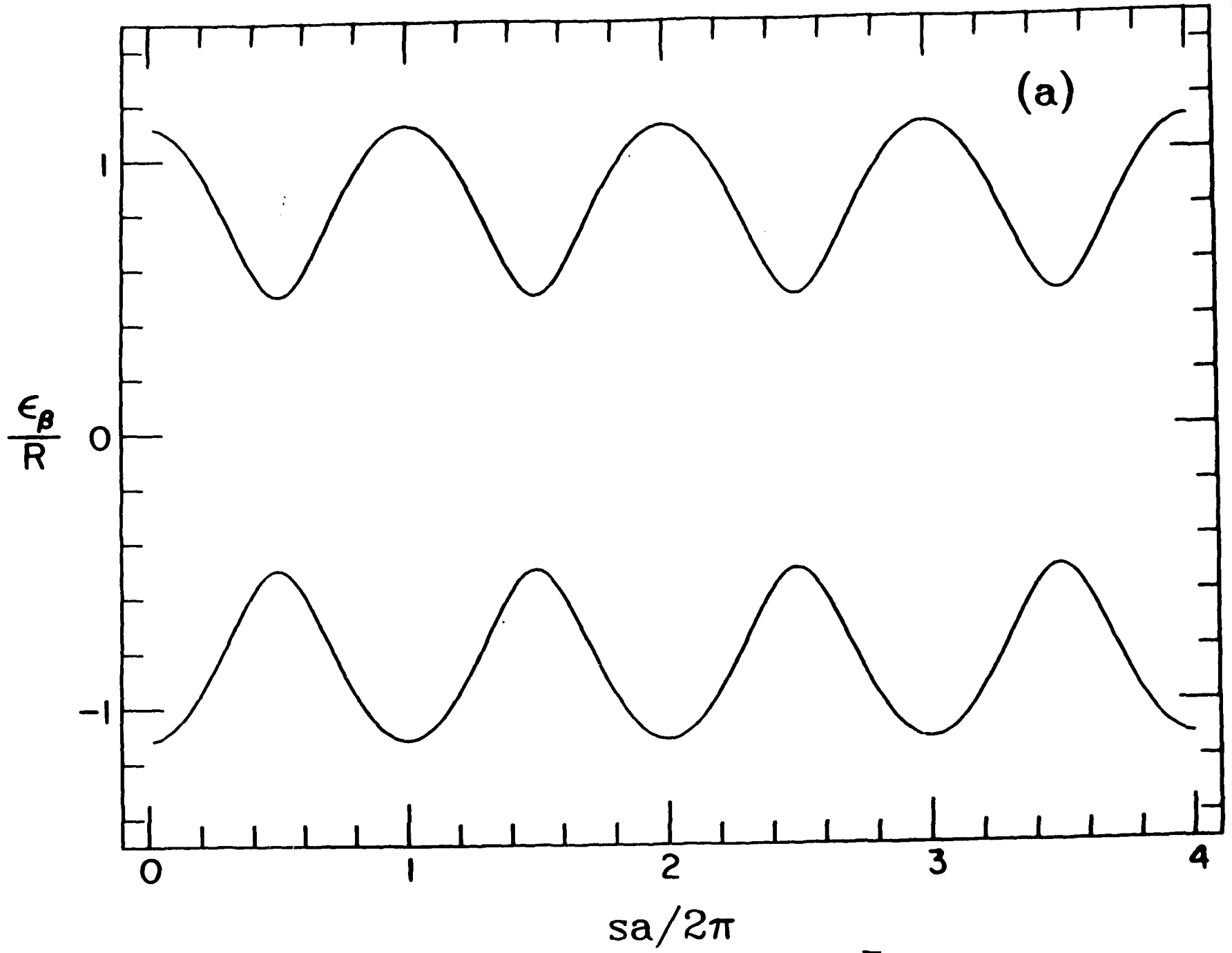


Fig. 2a

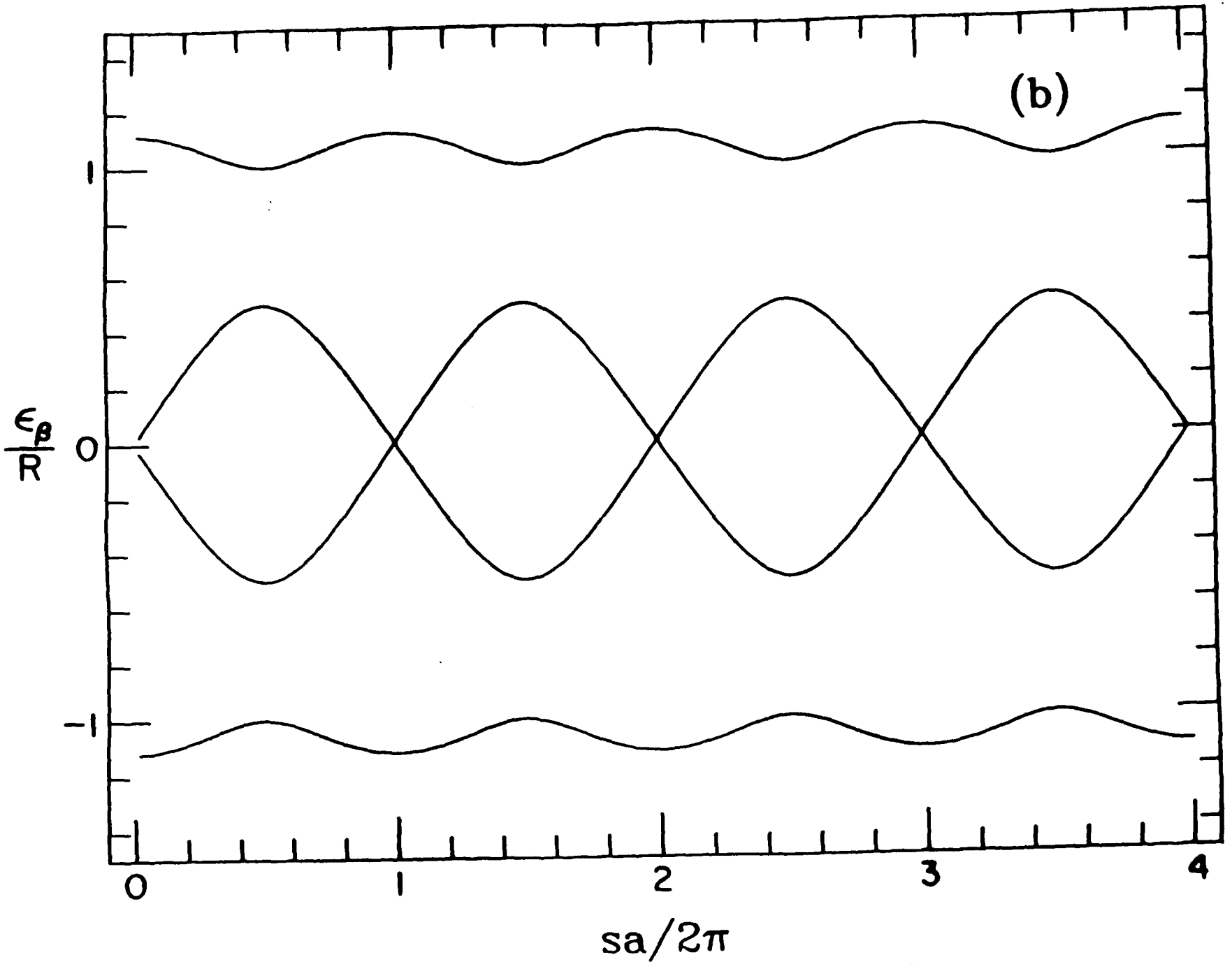
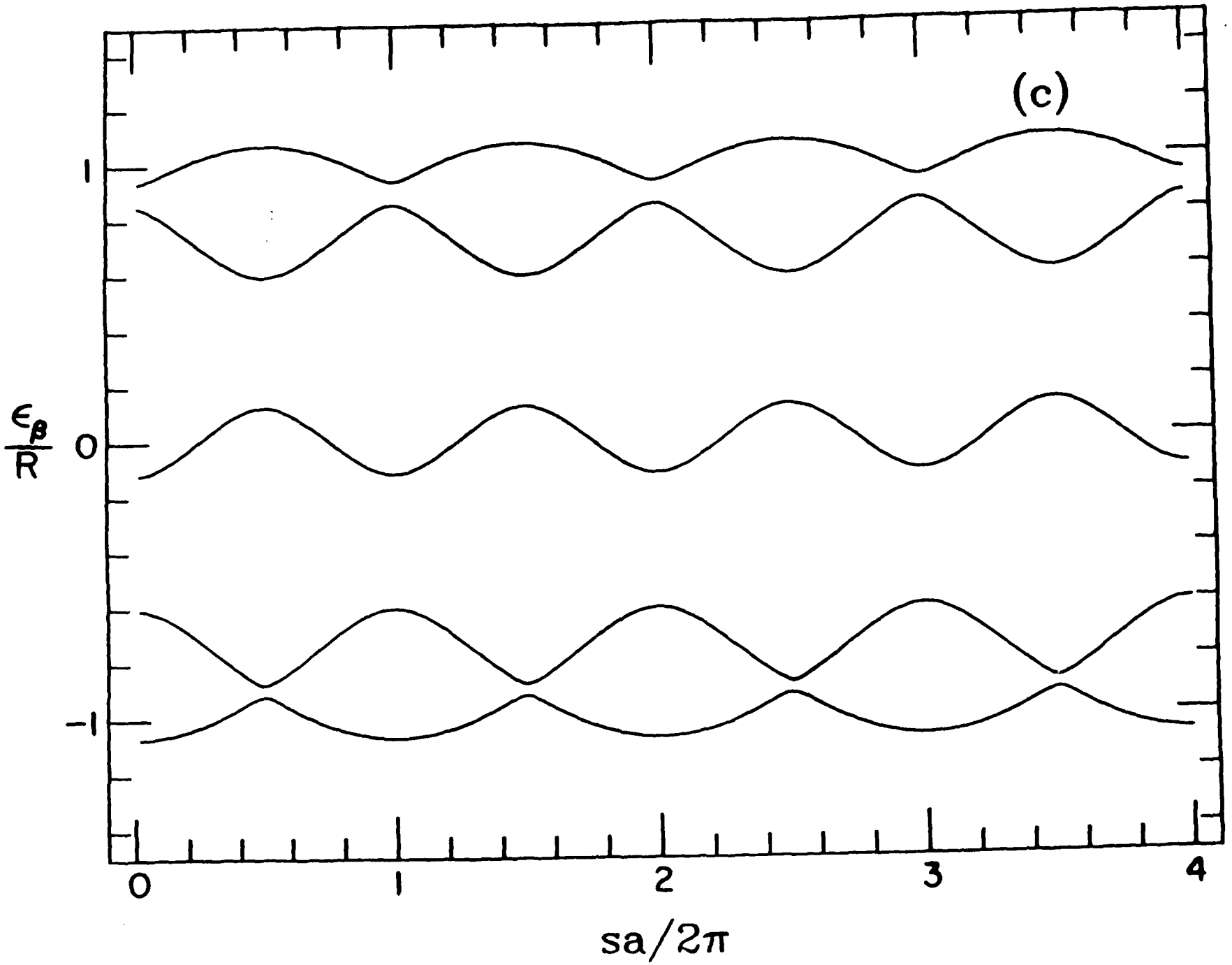


Fig. 2b



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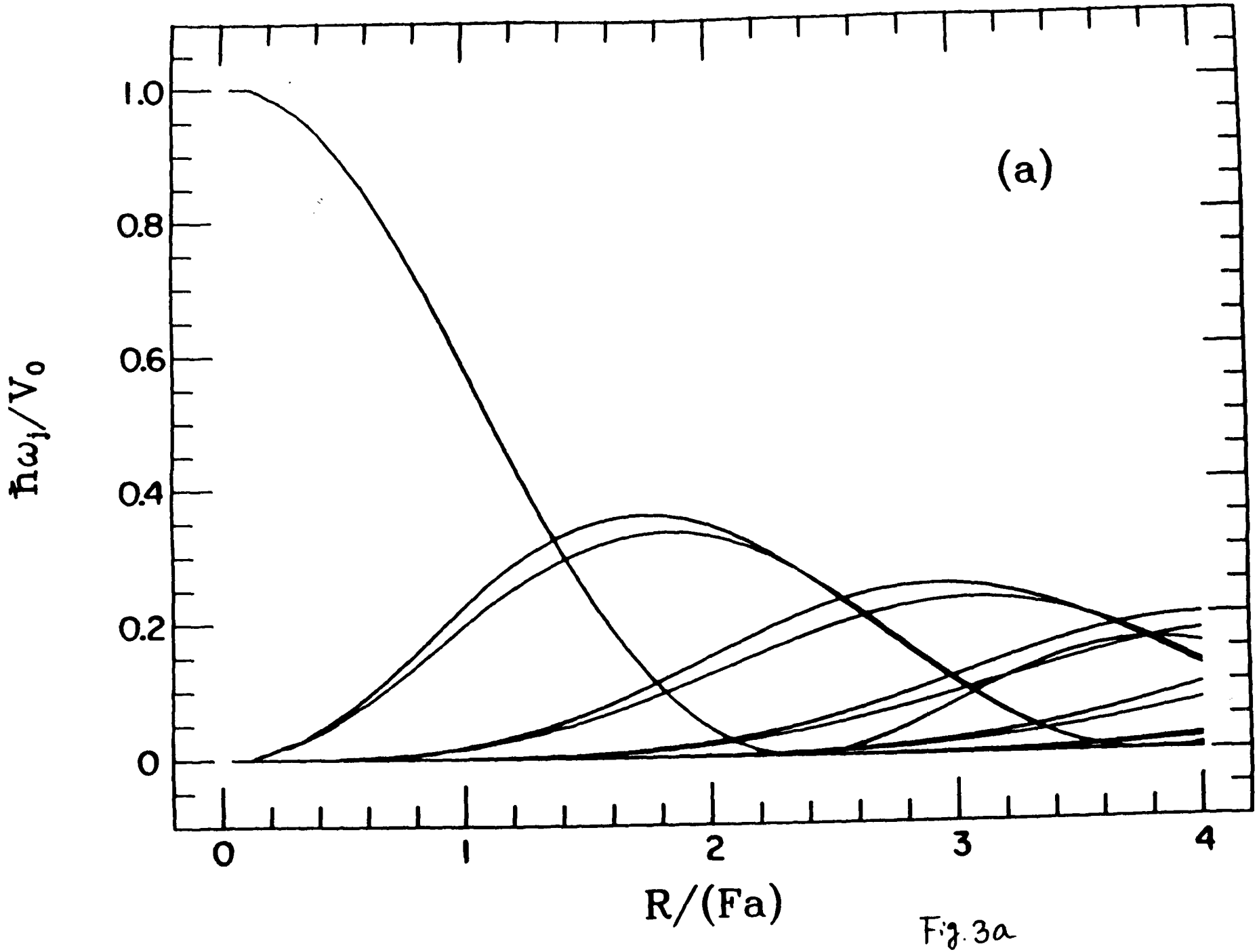

Fig. 3a

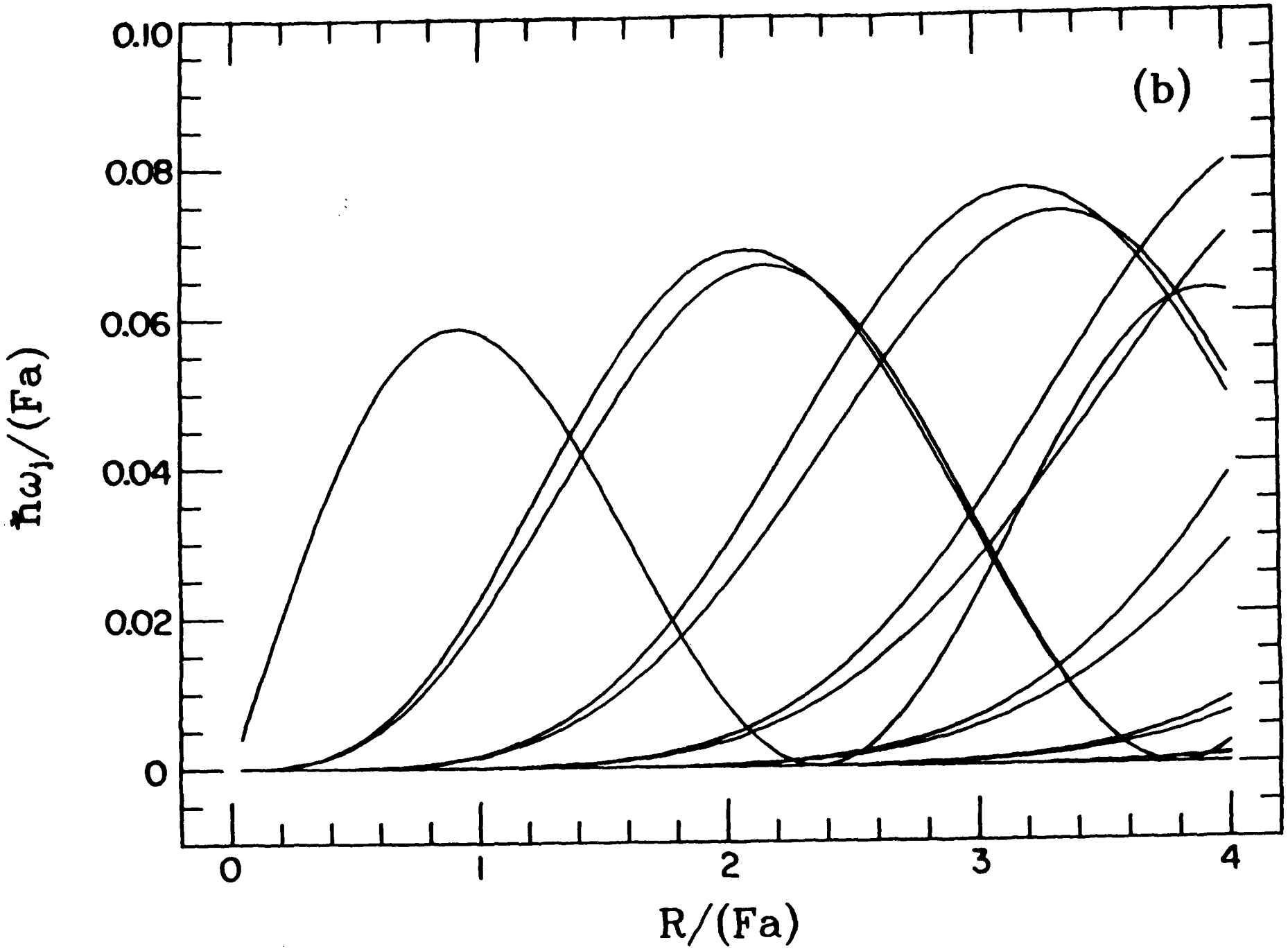

Fig. 3b